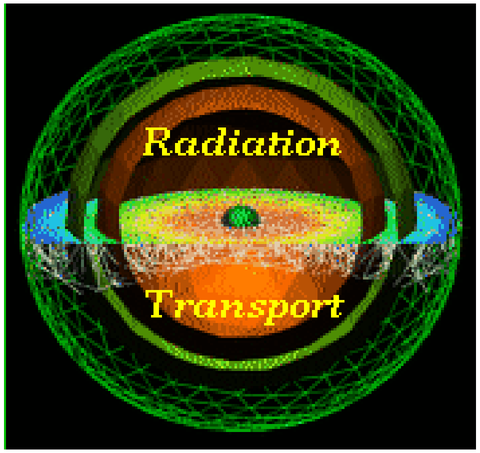

3-D Deterministic Transport Research at LANL under ASCI

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Overview

- **Research review**
- **Attila and Pericles Codes**
- **Three-dimensional unstructured-mesh neutral and charged particle transport calculations**
  - » **Fast Reactor (Takeda Benchmark Model 4)**
  - » **Gamma well-logging tool**
  - » **Reactor PV fluence**
  - » **RADPACK (Coupled Electron-photon, Silicon Chip Dose)**

Research Review

- **All ASCI transport research at LANL falls into one of the following two categories:**
  - » **Development of numerical methods for discretizing the transport equation and solving the discretized equations**
  - » **Development of parallel solution algorithms for applying numerical solution techniques in a parallel manner**

Research Review

- **ASCI research activities within the Transport Methods Group are organized into the following thrust areas:**
  - » **Parallel algorithms for the standard first-order form of the transport equation on rectangular meshes**
  - » **Numerical methods and parallel algorithms for second-order, self-adjoint forms of the transport equation on unstructured meshes**
  - » **Numerical methods and parallel algorithms for the standard first-order form of the transport equation on unstructured meshes**

Research Review

- Parallel S_n algorithms for 3-D rectangular meshes have been developed and implemented in the PARTISN code
  - » These methods are among the most effective that have ever been developed. For instance efficiencies on the order of 80 percent have been obtained with 3000 processors while retaining optimal single-processor performance
  - » This work has very recently been extended to block-refined rectangular meshes

Research Review

- **Both numerical methods and parallel algorithms have been developed for second-order forms of the transport equation on 3-D unstructured hybrid finite-element meshes**
  - » **Hybrid finite-element meshes consist of arbitrary combinations of hexahedra, wedges, pyramids and tetrahedra**
  - » **This work is more relevant to thermal radiative transfer than neutronics**
  - » **Both S_n and P_n calculations can be performed using this approach**

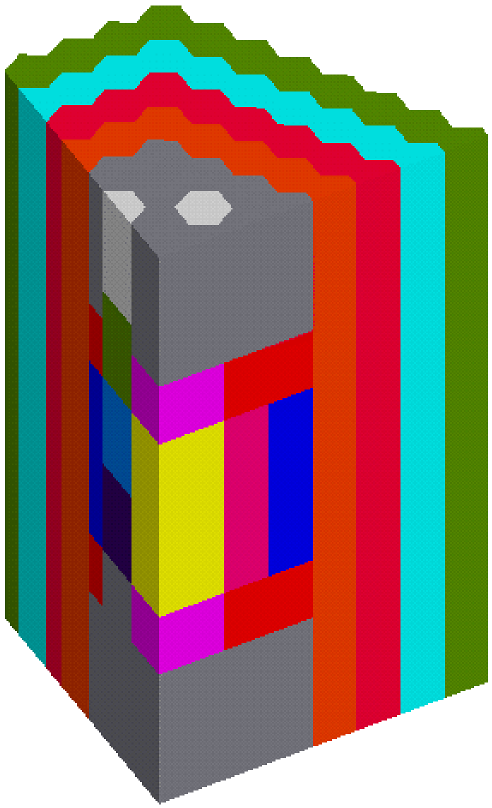
Research Review

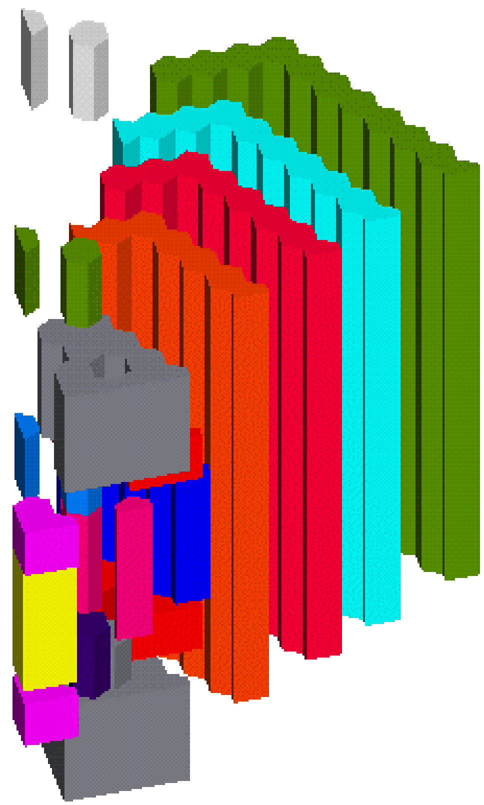
- **Numerical methods have been developed for the standard form of the S_n equations on 3-D unstructured tetrahedral and hexahedral meshes for neutral and charged particles.**
  - » **Long-term computational testing continues to indicate that these new S_n methods could have a major impact upon the state-of-the-art for transport calculations**
  - » **A parallel solution algorithm compatible with these new Sn methods has very recently been developed**

The Attila and Pericles Codes

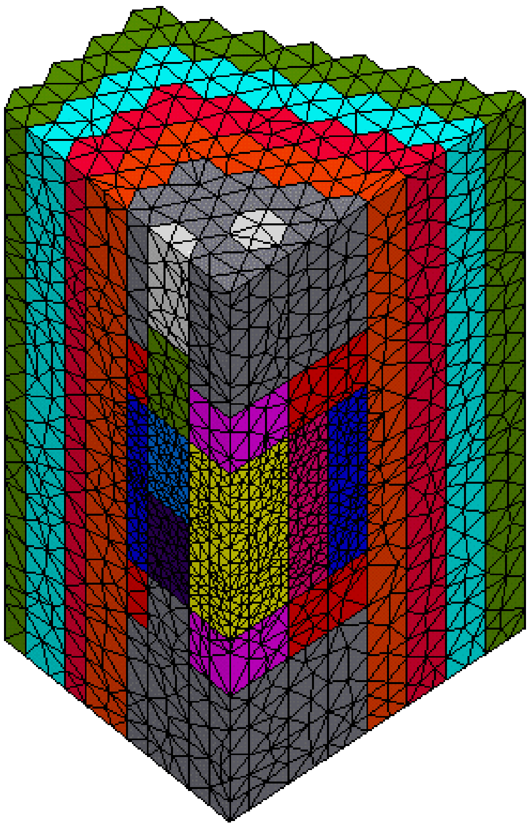
- **Attila**
  - » **First order 3-D unstructured tetrahedral mesh S_n code:**
  - » **Neutral and charged particles**
  - » **LD FEM spatial differencing**
  - » **LD FEM energy differencing of charged particle CSD operator.**
  - » **Diffusion synthetic acceleration of inner iterations.**
  - » **Forward or Adjoint modes.**
  - » **Other standard S_n code features.**
- **Pericles**
  - » **First order unstructured mesh S_n code.**
  - » **Same features as Attila with the addition of:**
    - – **1-D line meshes**
    - – **2-D triangle and quad meshes**
    - – **3-D tetrahedral and hexahedral meshes.**
  - » **We also have a time-dependent version of Pericles with LD FEM time differencing.**

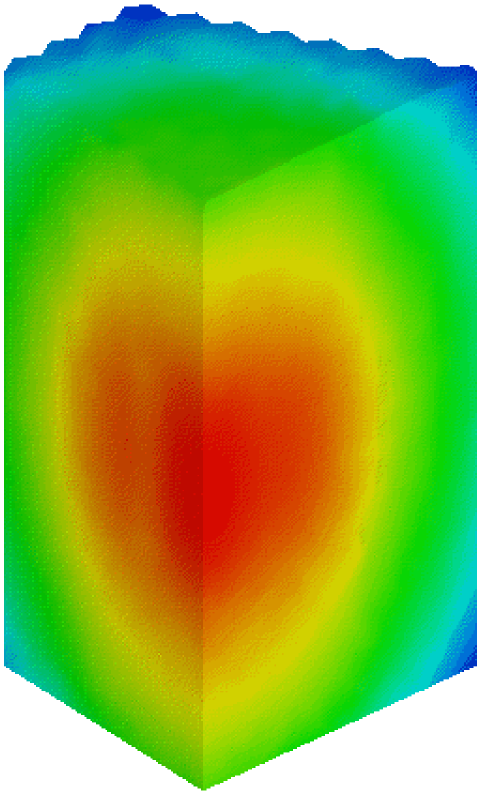
Fast Reactor





Fast Reactor





Mesh created by ICEM Tetra^{Tm}
52,092 Tets

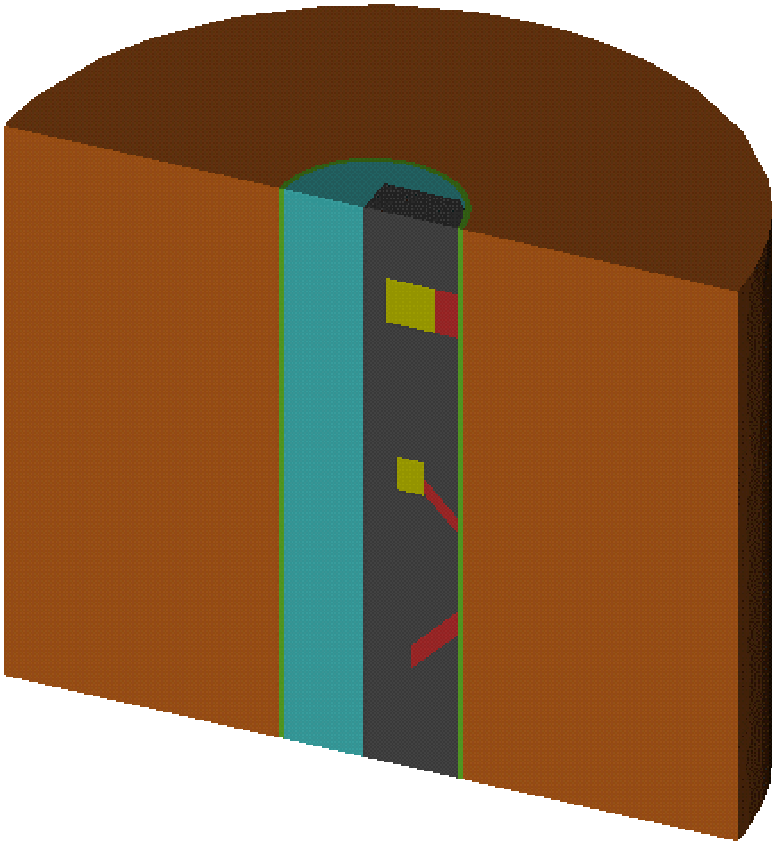
Fast Reactor

k_{eff}

Method	**Case 1** Control Rod Out	**Case 2** Control Rod Partly In	**Case 3** Control Rod In	Control Rod Worth
MC (reference)	1.0951 (.0004)	0.9833 (.0004)	0.8799 (.0003)	2.23E-1
Attila S_4	1.0948	0.9829	0.8791	2.24E-1
Attila S_8	1.0950	0.9831	0.8793	2.24E-1

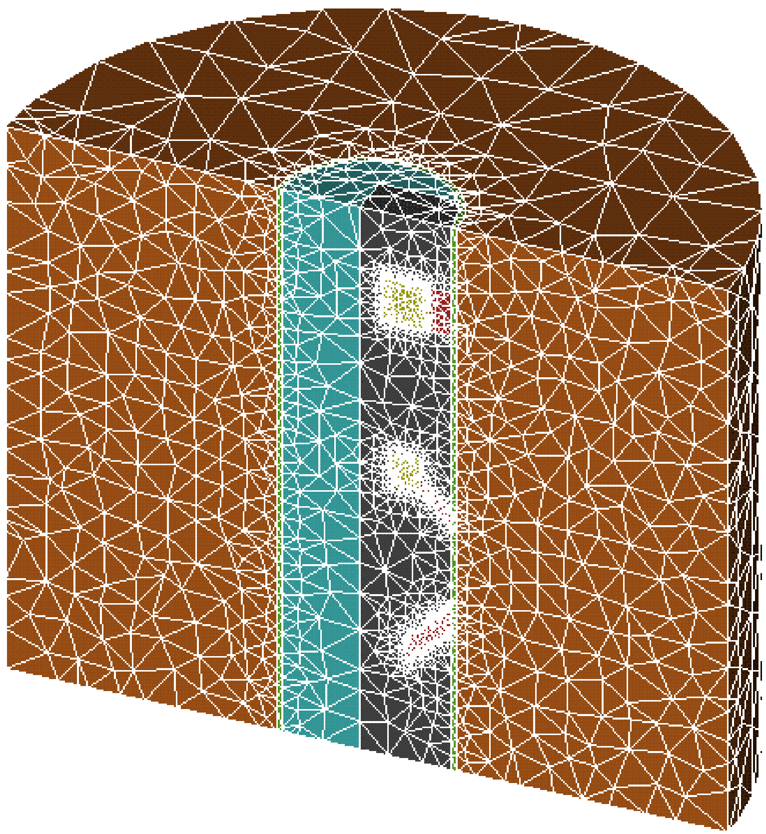
All calculations were performed on a 500 MHz Pentium III PC running under Linux. CPU Time were approximately 20 minutes and 60 minutes for S_4 and S_8, respectively

Gamma Well-Logging Tool



Gamma Well-Logging Tool

ICEM Tetra™ Grid
35,698 Tetrahedra
12 Energy Groups
S_{14} Quadrature
P_9 Scattering



Gamma Well-Logging Tool

Monte Carlo

$$\boxed{\ln(C_{near}) = (-0.309 \pm 5.35\%)r}$$

$$\boxed{\ln(C_{far}) = (-1.968 \pm 1.24\%)r}$$

➡ **50+ CPU hours on SGI Octane**

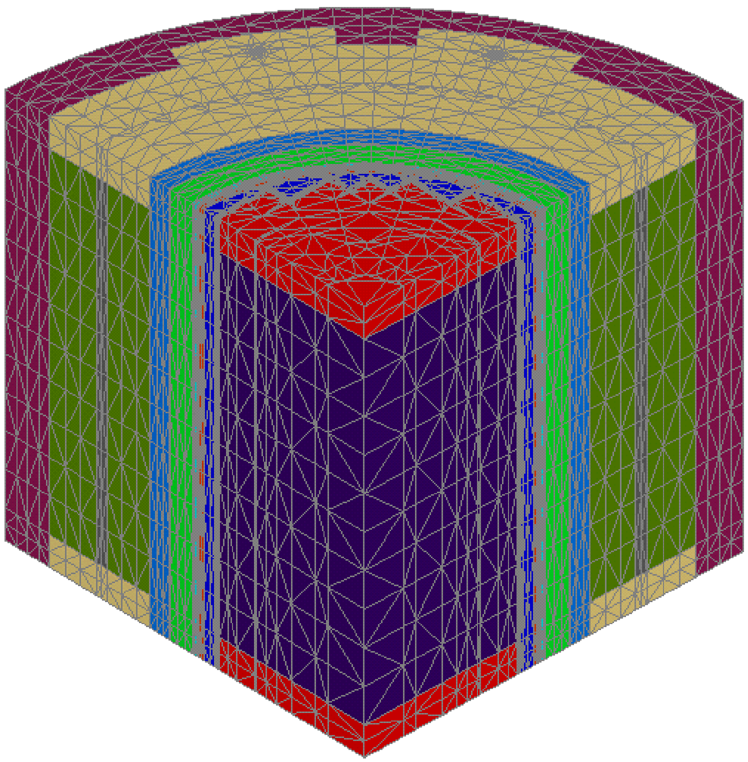
Attila

$$\boxed{\ln(C_{near}) = (-0.313)r}$$

$$\boxed{\ln(C_{far}) = (-1.961)r}$$

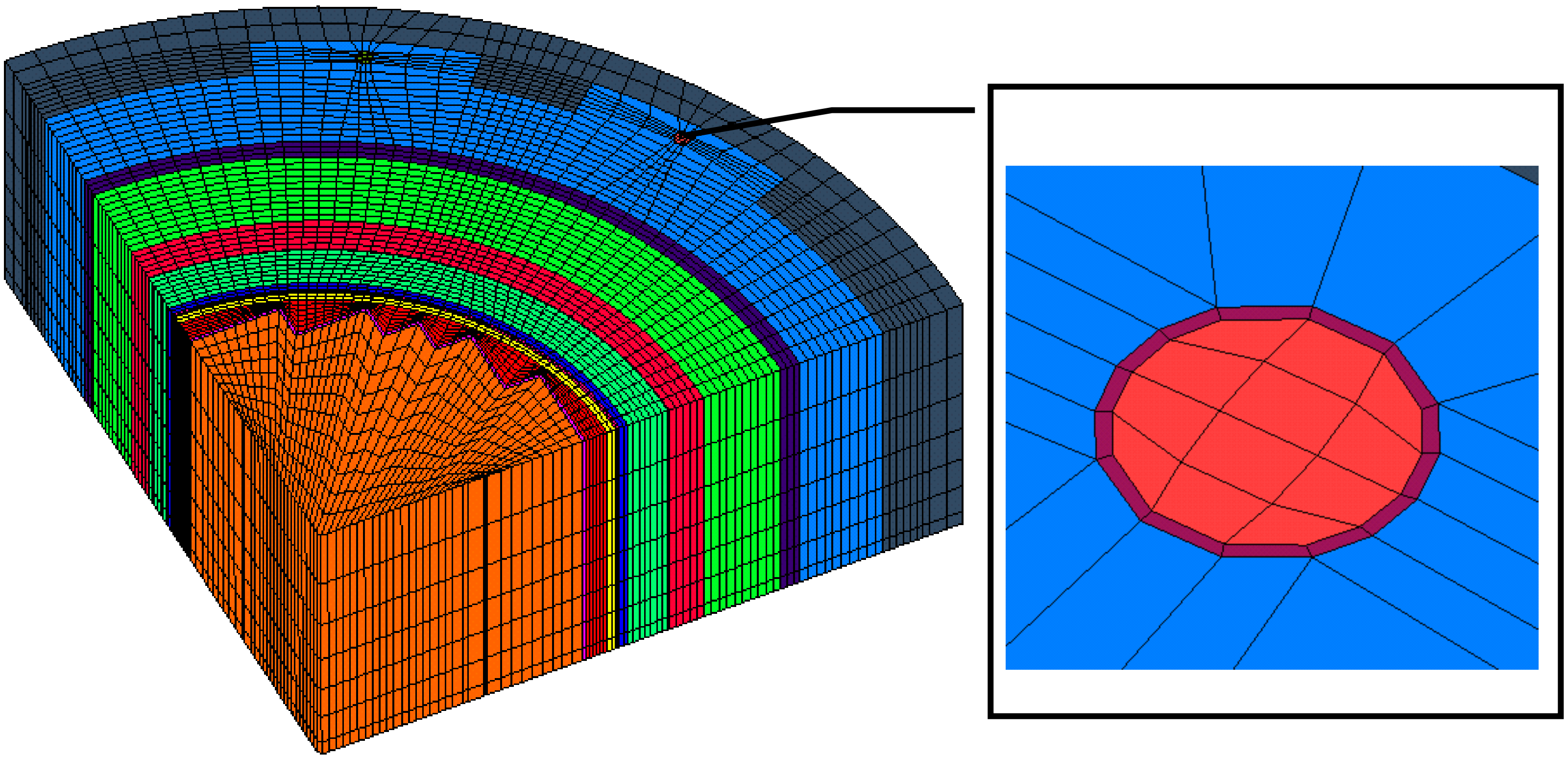
➡ **12 CPU hours on SGI Octane**

Reactor PV Fluence



Six detector locations specified. Mesh contains ~90,000 tets.
Attila S_8/P_3 , 26 group results matched the MC results to within 10 %.
The calculations required ~ 20 hours on Sun Ultra 2 (slower machine by today's standards).

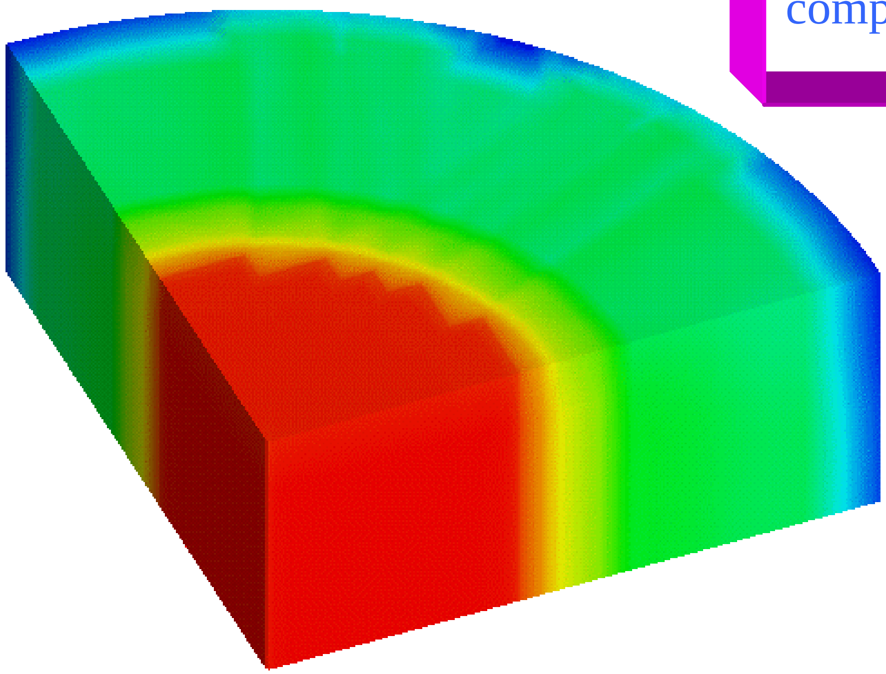
Reactor PV Fluence



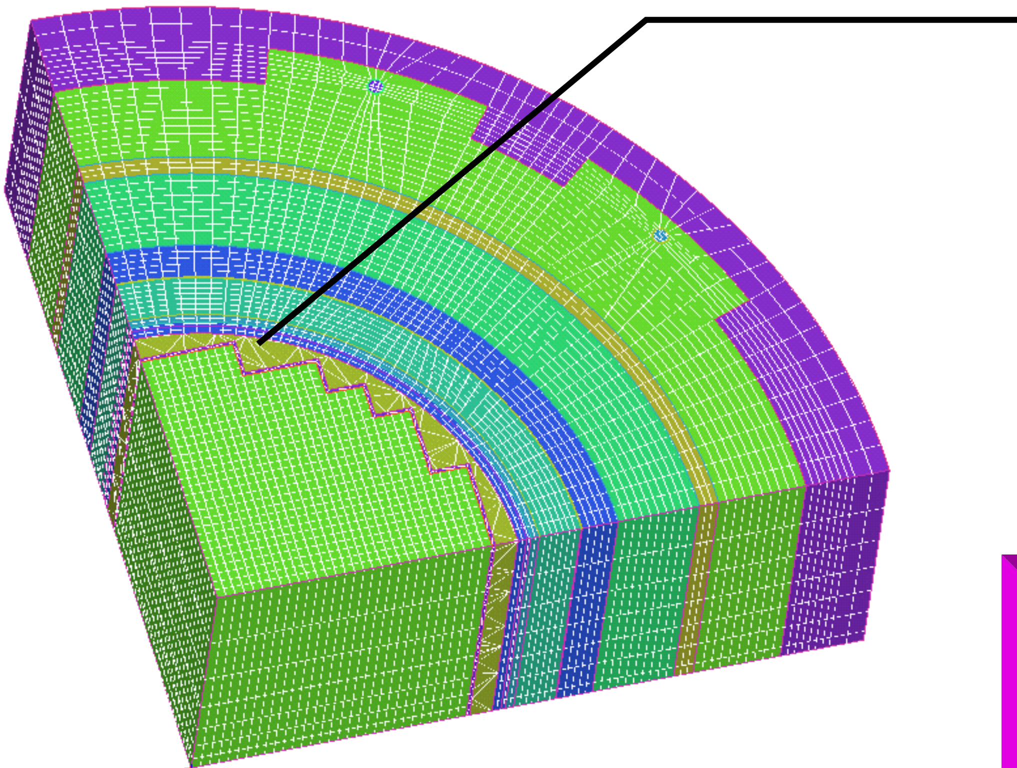
ICEM Hexa^{TM} Grid
20,664 Hexes

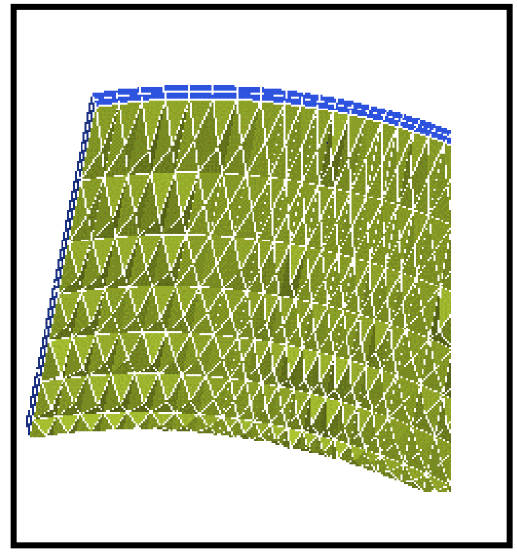
Reactor PV Fluence

The calculations required ~ 5 hours on 500 MHz PC under Linux and were comparable to the tet mesh solutions.



Reactor PV Fluence

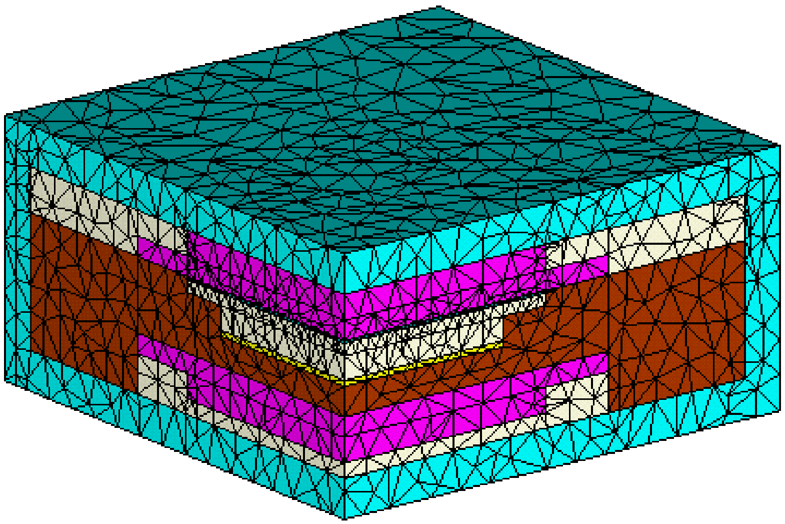




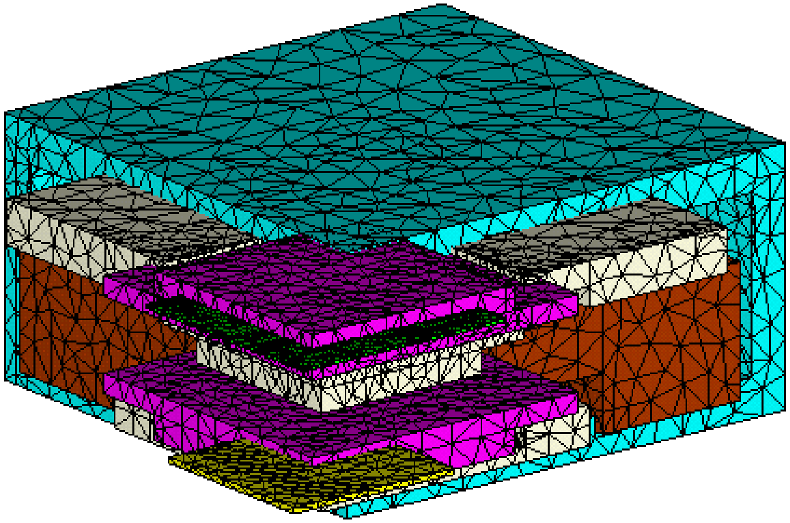
Merged ICEM Hexa™ and Tetra™ Grid
20,503 Hexes, 7,476 Tets and 456 Pyras

We have the technology to run true hybrid meshes and this capability will be in our next generation codes.

RADPACK Coupled Electron-Photon

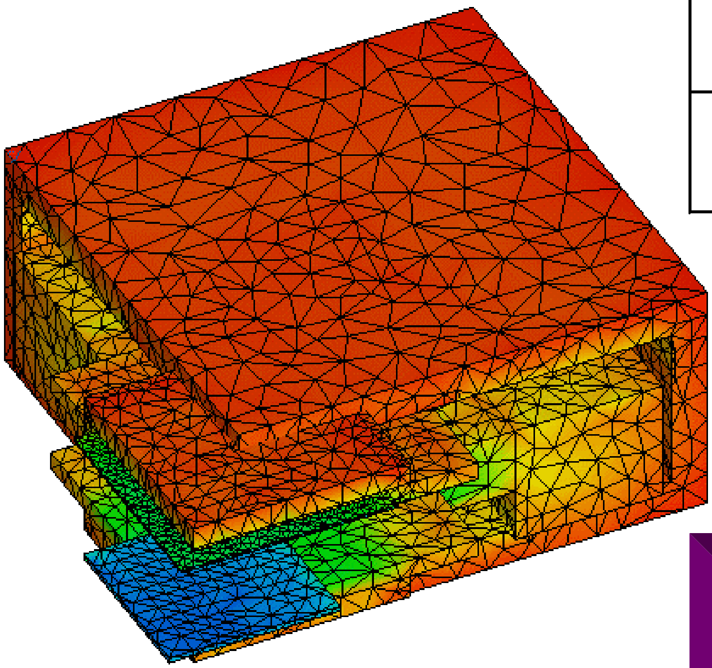


ICEM Tetra™ Grid
51,963 tetrahedra
30 electron groups
10 photon groups
S_4 galerkin quadrature
P_5 scattering



RADPACK Coupled Electron-Photon

Method	RAD S (Primary e^-)	RAD S (Brems.)	RAD S Total
MC (ITS) (1984)	3.36E-11 (14%)	8.40E-12 (7%)	4.21E-11 (11%)
Attila (Attila/MC)	3.58E-11 (1.07)	8.61E-12 (1.03)	4.44E-11 (1.05)



The calculations required ~ 5.3 hours on 500 MHz PC under Linux